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Air Quality Data Analysis System for Interrelating Effects, Standards, and Needed Source Reductions. Part 9. Calculating Effective Ambient Air Quality Parameters

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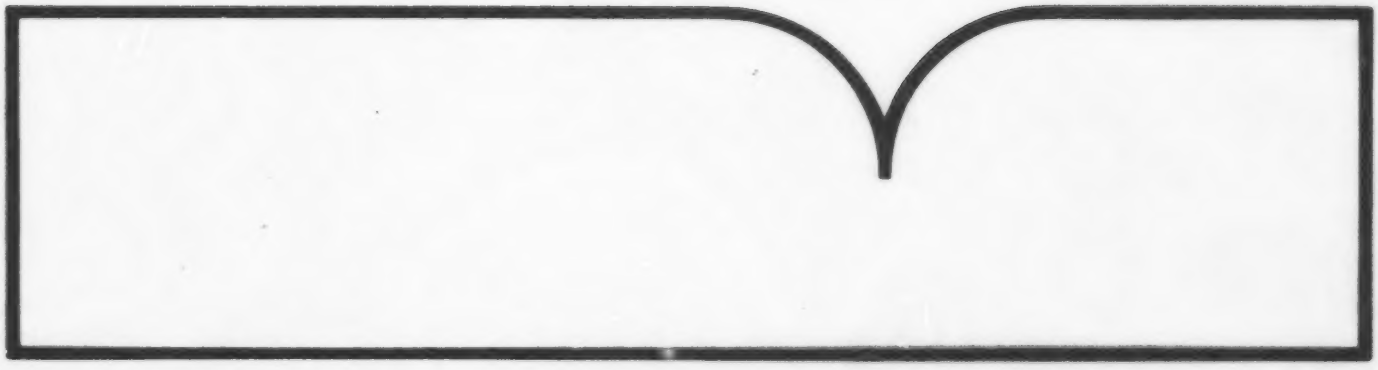

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16. ABSTRACT The overall purpose of air pollution control is to reduce or eliminate adverse effects, such as plant injury or crop reduction. In order to study and to control such adverse effects efficiently, air quality parameters are needed that correlate closely with the effects. One such air quality parameter is the effective mean concentration:

$$m_e = [(\Sigma\ c_h^{-1/v})/n]^{-v}$$

where c_h is the 1-h average ambient air pollutant concentration measured at a site for each daytime hour (defined here as 9:00 A.M.-4:00 P.M., always standard time) in a plant's growing season, n is the number of hours of such available data, and v is a concentration-time parameter (-0.376 is always used here). Ambient air quality data can often be characterized by the two characteristic parameters of the lognormal distribution, the geometric mean and the standard geometric deviation, but some ambient data are far from lognormal. This paper suggests that even though an air quality data set is not lognormal, the effects of the concentrations can be characterized with an effective geometric mean and an effective standard geometric deviation calculated from the effective and arithmetic means. These two effective parameters can be used to characterize air quality at a site, in terms of its expected effects on plants, and to compare these parameters and the expected plant effects from site to site.

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An Air Quality Data Analysis System for Interrelating Effects, Standards, and Needed Source Reductions: Part 9. Calculating Effective Ambient Air Quality Parameters

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The overall purpose of air pollution control is to reduce or eliminate adverse effects, such as plant injury or crop reduction. In order to study and to control such adverse effects efficiently, air quality parameters are needed that correlate closely with the effects, as does the effective mean concentration:

$$m_e = [(\sum c_h^{-1/v})/n]^{-v},$$

where c_h is the 1-h average ambient air pollutant concentration measured at a site for each daytime hour (defined here as 9:00 A.M.–4:00 P.M., always standard time) in a plant's growing season, n is the number of hours of such available data, and v is a concentration-time parameter (−0.376 is always used here, based on previous studies). Ambient air quality data can often be characterized by the two characteristic parameters of the lognormal distribution, the geometric mean and the standard geometric deviation, but some ambient data are far from lognormal. This paper suggests that even though an air quality data set is not lognormal, the effects of the concentrations can be characterized with an effective geometric mean, m_{gee}, and an effective standard geometric deviation, s_{gee}, calculated from the effective and arithmetic means:

$$m_{gee} = (m_e m_a^{1/v})^{1/(1+1/v)}, \; s_{gee} = \exp|[2 \ln(m_a/m_{gee})]^{0.5}|,$$

where exp indicates that e, 2.718, is raised to the power in brackets. These two effective parameters can be used to characterize air quality at a site, in terms of its expected effects on plants, and to compare these parameters and the expected plant effects from site to site.

The overall purpose of air pollution control is to reduce or eliminate the adverse effects of air pollutants on people, animals, plants, and property. The air pollution control sequence begins with the publication of air quality criteria documents that list adverse effects and their associated air pollutant concentration parameters (e.g., means and maxima for various averaging times). National Ambient Air Quality Standards (NAAQS) are developed from these criteria. Emission standards are then developed and applied to achieve the NAAQS.

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Estimating Plant Effects with the Effective Mean and Impact Parameters

Although air quality parameters associated with various adverse effects are listed in criteria documents, questions often arise concerning which air quality parameter correlates best with each effect. Is an effect due primarily to a long term mean, a short term maximum, or to repeated exposures to varying ambient concentrations above a threshold concentration? The two preceding papers in this series[1, 2] suggest that several types of plant effects correlate well with a new air pollutant parameter called total impact, which gives greater weight to the higher concentrations measured during a plant's exposure. The impact parameter is based on analyses of the amount of leaf injury, growth suppression, or leaf dry weight reduction measured during acute and chronic exposures of plants to O_3.

The hourly impact is defined as an hour's pollutant concentration raised to an exponent:

$$I_h = c_h^{-1/v} \quad (1)$$

where v = the slope of equal effects isopleth lines on a logarithmic plot with pollutant concentration on the ordinate and exposure time on the abscissa (e.g., Figure 1).

Total impact is the summation, over a plant's growing season, of each daytime (9:00 A.M.-4:00 P.M.) hour's pollutant concentration raised to an exponent:

$$I_t = \sum c_h^{-1/v}. \quad (2)$$

Another new parameter, the effective mean concentration, is derived from impact. It is the mean of the hourly impacts raised to the $-v$ power:

$$m_e = [(\sum c_h^{-1/v})n]^{-v}. \quad (3)$$

If v were -1, the effective mean would equal the arithmetic mean. The studies of O_3 plant effects mentioned above suggest a v approximating -0.376. The negative reciprocal, $-1/v$, is 2.66. These two values are used throughout this paper.

One example application of the effective mean O_3 concentration is an equation developed previously to estimate soybean crop reduction:[2]

$$z = 0.478 \ln (t m_e^{2.66}) - 0.42 \quad (4)$$

where z = the Gaussian transform of percent crop reduction; e.g., the number of standard deviations (right side of Figure 1) that a percent effect (left side of Figure 1) is located away from the median (50%),

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t = the hours of exposure (525 h; 7 h/day for 75 days), and

ln = the natural logarithm (of the quantity within parentheses).

If a concentration value is available for each exposure hour, then Equations 2–4 indicate that

$$I_t = t m_e^{2.66}. \quad (5)$$

Using this relationship, Equation 4 can be expressed as

$$z = 0.478 \ln I_t - 0.42. \quad (6)$$

Mathematical Modeling Assumptions

The mathematical modeling that follows is analagous to building a concrete bridge: forms are built, concrete is poured into the forms, then the forms are removed, leaving a free-standing bridge. The development here is easiest to follow if judgment about the "forms" is withheld until the end. The "forms" assumptions are:

1. The effective mean air pollutant concentration (Equation 3) measured at any air sampling site correlates well with crop reduction (Equation 4).
2. One hypothetical air sampling site exists where 1-h average air pollutant concentrations fit a lognormal frequency distribution perfectly and that distribution can therefore be completely described with two parameters: the geometric mean, m_{ga}, the concentration exceeded 50 percent of the time; and the standard geometric deviation, s_{ga}, the concentration exceeded 16 percent of the time divided by the concentration exceeded 50 percent of the time.
3. Because concentration is lognormally distributed, ln c_h is normally distributed.
4. The logarithm of an hourly impact (Equation 1) can be expressed either as ln $(c_h^{-1/v})$ or $-1/v$ ln c_h. Because concentration is lognormally distributed, impact is also lognormally distributed.
5. The two characteristic parameters of a lognormal frequency distribution, m_{ga} and s_{ga}, can be calculated (as will be shown) from the effective mean, m_e, and the arithmetic mean, m_a, of a perfectly lognormal set of air pollutant concentration data.
6. Now switch from a perfectly lognormal set of ambient air quality data to any set of ambient air quality data, no matter how it is distributed. The effective ambient geometric mean, m_{gae}, and the effective ambient standard geometric deviation, s_{gae}, are defined and calculated exactly the same as m_{ga} and s_{ga} in Assumption 5. Conversely m_e and m_a can be calculated from m_{gae} and s_{gae}. Because of the definitions in Assumptions 5 and 6, these last four parameters always can be computed (unless $v = -1$), no matter how poorly a concentration distribution fits lognormality. Because our only interest here is to express crop reduction as a function of the effective mean concentration (Assumption 1), any two of these four parameters will suffice. Estimated crop reduction will be expressed here, as an example, as a function of the arithmetic mean O_3 concentration and the effective ambient standard geometric deviation (Figure 3).
7. The m_{gae} and s_{gae} parameters are consistent with m_e and m_a for any air quality data set, as defined above. This paper is concerned only with these four parameters, not with the goodness-of-fit to lognormality for any other parts of any air quality distribution.

Characterizing Ambient Air Quality with an Effective Geometric Mean and an Effective Standard Geometric Deviation

Having stated the assumptions, equation development and calculations can proceed. The concentration indicated for the eight lowest hourly O_3 concentrations in Table I, 0.002 ppm, is really 0.000 ppm in the National Aerometric Data Bank (NADB) and is used here as 0.000 when calculat-

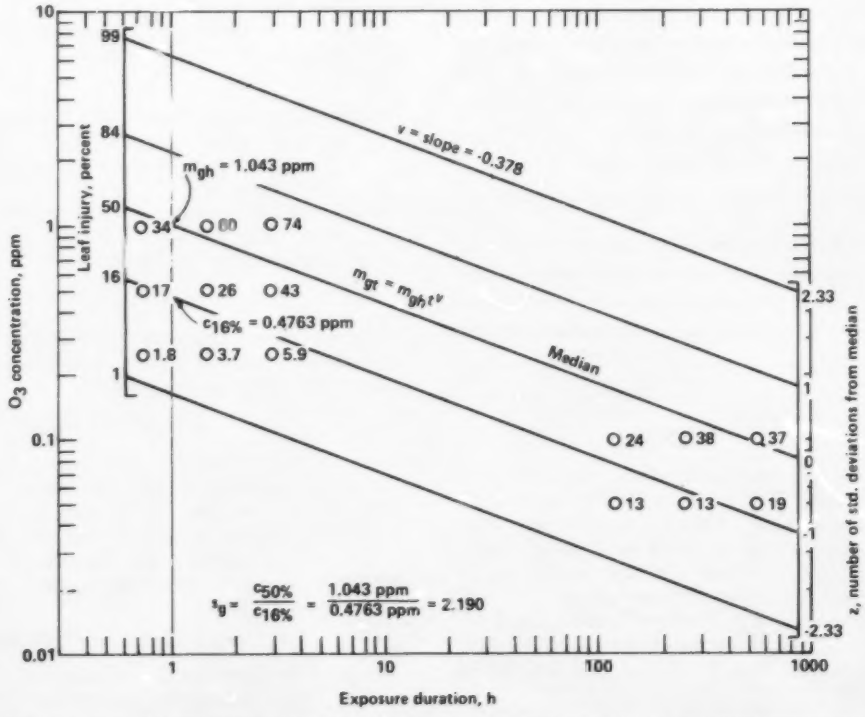

Figure 1. Percent leaf injury in Lee 68 and Dare soybeans exposed acutely (for 0.75, 1.5, or 3 h) and Dare soybean exposed chronically (for 120, 258, or 552 h) to O_3.[2]

ing the arithmetic and effective means. The concentration is used here as 0.002 (taken here as 40 percent of the lowest non-zero recorded concentration, in order to give an even ppb) only for later calculations involving logarithms, because logarithms cannot be taken of zero.

The data (Table I) were plotted (Figure 2). Each group of hours with the same hourly O_3 concentration (column 1) and their hourly impact (column 5) were plotted on log-probability cumulative frequency distribution graph paper, at the frequency listed (colum 3), by using the equation that will be used in later truncation calculations:[3]

$$f = (100)(r - 0.5)/n \qquad (7)$$

where f = the plotting frequency in percent,
r = the rank of the midpoint of a sample group, and
n = the total number of samples available.

Using Equation 7, the one 0.070 ppm sample has a rank of 9 and a plotting frequency of 1.389 percent. The four 0.090 ppm samples have a midpoint rank of 2.5 and a plotting frequency of 0.327 percent.

If concentration data from an air sampling site are perfectly (Assumption 2) lognormally distributed (they will form a perfectly straight line on Figure 2), the interrelation among parameters (Equation 2.7 in Reference 4) is

$$\ln m_a = \ln m_{ga} + 0.5 \ln^2 s_{ga} \qquad (8)$$

where m_a = the ambient arithmetic mean concentration,
m_{ga} = the ambient geometric mean concentration, and
s_{ga} = the ambient standard geometric deviation.

Because the hourly impact of each 1-h average air pollutant concentration is defined here as

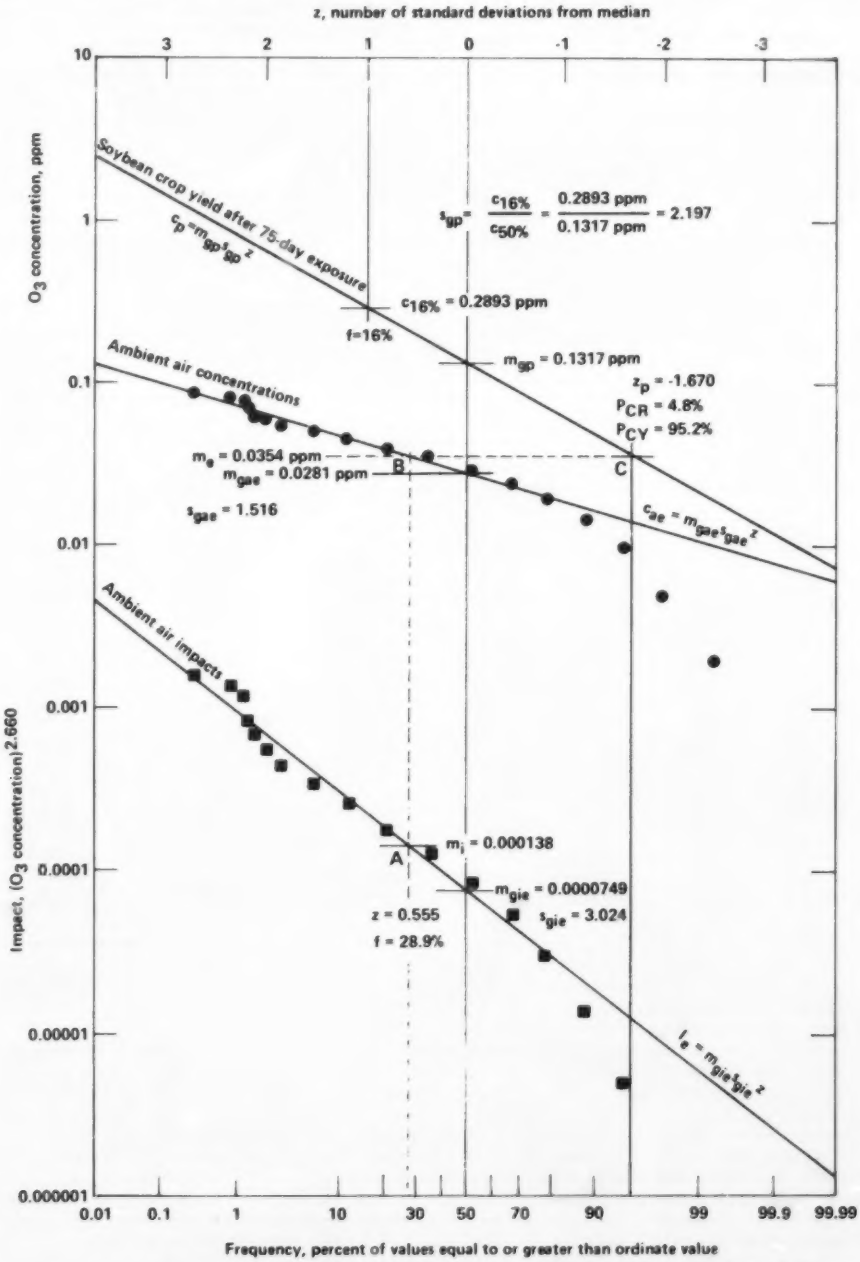

Figure 2. Cumulative frequency distributions of 1-h average O_3 concentrations, impacts, and estimated soybean crop yields for daytime (9:00 A.M.–4:00 P.M.) during summer (June 1–August 31) of 1981 at NADB site 262950001A08, Cottoner Mountain National Forest Station, Mark Twain National Forest, Madison County, Missouri.

$$I_h = c_h^{-1/v} \quad (1)$$

then

$$m_{gi} = m_{ga}^{-1/v} \quad (9)$$

$$s_{gi} = s_{ga}^{-1/v} \quad (10)$$

where subscript i indicates an impact parameter and subscript a indicates an ambient air pollutant concentration parameter (Equation 8). The hourly impacts, as well as the hourly concentration data, are perfectly lognormally distributed (Assumption 4):

$$\ln m_i = \ln m_{gi} + 0.5 \ln^2 s_{gi} \quad (11)$$

where m_i = the arithmetic mean of the hourly impacts.

The ambient effective mean pollutant concentration defined above (Equation 3) can also be expressed as

$$m_e = m_i^{-v}. \quad (12)$$

Taking natural logarithms and solving for $\ln m_i$

$$\ln m_i = (1/-v) \ln m_e. \quad (13)$$

Using the above relationships, the m_{ga} parameter can be expressed as a function of m_a, m_e, and v by taking the following steps: substitute Equation 13 into Equation 11; apply Equations 9, 10; use Equation 3 to replace the s_{ga} term; solve for $\ln m_{ga}$; take antilogarithms; and define m_{ga} as an effective parameter, m_{gae} (Assumption 6):

$$m_{gae} = (m_e m_a^{1/v})^{1/(1+1/v)}. \quad (14)$$

Using $v = -0.376$,

$$m_{gae} = (m_e m_a^{-2.660})^{-0.6026}. \quad (15)$$

Equation 8 can be rearranged to solve for s_{gae}.

$$s_{gae} = \exp\{[2 \ln (m_a/m_{gae})]^{0.5}\} \quad (16)$$

The effective mean of 0.0354 ppm (bottom of Table I) was calculated (Equation 12) from the mean impact of 0.000138 (bottom of column 5). The effective and arithmetic means were then used to calculate (Equations 14, 16) the effective ambient geometric mean of 0.0281 ppm and the effective ambient standard geometric deviation of 1.516.

Comparing Effective Parameters with Traditional and Truncated Parameters

To enable comparisons, the two characteristic parameters of a lognormal frequency distribution, the geometric mean and the standard geometric deviation, were calculated by three methods and listed at the bottom of Table I. The three sets of values are separated from each other by horizontal lines. In the last set, the two characteristic parameters were calculated by the traditional method: the logarithm of each concentration value was taken, the mean and standard devi-

Table I. Frequency distribution, concentration parameters, and estimated crop reduction for soybeans exposed for 75 days during the summer (June 1–August 31) of 1981 to ambient daytime (9:00 A.M.–4:00 P.M.) 1-h average O_3 concentrations (data available for 95% of the hours) at NADB site 262950001A08, Cottoner Mountain National Forest Station, Mark Twain National Forest, Madison County, Missouri.

Conc, ppm (1)	Number of h (2)	Plotting position: Freq, % (3)	Plotting position: z (4)	Impact: For 1 h (5)	Impact: For all h (6)	Impact: Cumulative (7)	Cumulative crop reduction, % (8)	Cumulative air parameters: m_{ga}, ppm (9)	Cumulative air parameters: s_{ga} (10)
.090	4	.327	2.720	.001655	.006619	.006619	.2		
.085	3	.899	2.367	.001421	.004264	.010883	.5	.0580	1.176
.080	1	1.225	2.249	.001210	.001210	.012093	.6	.0512	1.232
.070	1	1.389	2.201	.000848	.000848	.012941	.6	.0338	1.447
.065	2	1.634	2.136	.000696	.001393	.014334	.7	.0224	1.697
.060	4	2.124	2.029	.000563	.002251	.016585	.9	.0172	1.882
.055	8	3.105	1.866	.000447	.003573	.020158	1.1	.0164	1.918
.050	29	6.127	1.544	.000347	.010051	.030209	1.8	.0215	1.708
.045	41	11.846	1.183	.000262	.010737	.040946	2.6	.0257	1.567
.040	76	21.405	.792	.000191	.014551	.055497	3.6	.0288	1.471
.035	90	34.967	.386	.000134	.012080	.067578	4.4	.0300	1.433
.030	112	51.471	-.037	.000089	.009977	.077555	5.1	.0302	1.424
.025	84	67.484	-.453	.000055	.004608	.082163	5.4	.0299	1.438
.020	57	79.003	-.806	.000030	.001727	.083890	5.5	.0294	1.474
.015	52	87.908	-1.171	.000014	.000733	.084623	5.5	.0286	1.537
.010	26	94.281	-1.579	.000005	.000125	.084748	5.5	.0280	1.599
.005	14	97.549	-1.969	.000001	.000011	.084758	5.5	.0275	1.690
.002	8	99.346	-2.482	.000000	.000000	.084758	5.5	.0270	1.799

n = 612 Mean impact = .000138 75-day crop reduction = 4.8%

.0307	Arithmetic mean concentration
.0354	Effective mean concentration
.0281	Effective geometric mean concentration (calculated from arithmetic and effective means)
1.516	Effective standard geometric deviation (calculated from arithmetic and effective means)
5	Percent crop reduction expected after a 75-day exposure to above effective mean concentration
.0294	Geometric mean concentration (calculated from pollutant concentrations > 0.019 ppm)
1.474	Standard geometric deviation (calculated from pollutant concentrations > 0.019 ppm)
.0359	Effective mean concentration (estimated from last 2 lines)
5	Percent crop reduction expected after a 75-day exposure to above effective mean concentration
.0270	Geometric mean concentration (calculated from all pollutant concentrations)
1.782	Standard geometric deviation (calculated from all pollutant concentrations)
.0421	Effective mean concentration (estimated from last 2 lines)
7	Percent crop reduction expected after a 75-day exposure to above effective mean concentration

ation of the logarithms were calculated, and the results were translated into a geometric mean and a standard geometric deviation. The chief drawback of this method for the data plotted is the effect of the lowest 15 percent of the concentrations. They contribute only 1 percent of the total impact (Table I column 7) but affect calculation of the two characteristic parameters just as much as the top 15 percent of the samples. The top 15 percent contributes almost half of the total impact. These calculations demonstrate the importance of carefully considering the expected effects of the high concentrations and not being very concerned about the low concentrations when fitting an "effective" frequency distribution.

If the lowest O_3 concentrations are truncated from the distribution, parameters are calculated[3] (second set at the bottom of Table I) that are nearer the effective parameters. Parameters calculated by truncation (Table I, columns 9, 10) are shown for each successive line. All the data above and on each line (in columns 1–4) were used to calculate the two characteristic parameters for that line. When concentrations below 0.020 ppm are truncated, the geometric mean and the standard geometric deviation are quite close to the values calculated from the arithmetic and effective means (first set of values). (The traditional and truncated methods both give the same geometric mean and almost the same standard geometric deviation, 1.78 vs. 1.80, if all data are included in the truncation calculations.)

Comparing Crop Reductions Estimated with Three Sets of Characteristics Parameters

A cumulative crop reduction of 5.5 percent (Table I, column 8) was calculated (Equation 6) for the 95 percent of daytime summer hours for which O_3 concentration data were available. If soybeans are exposed for 75 rather than 92 days, a crop reduction of 4.8 percent is calculated (Equation 4).

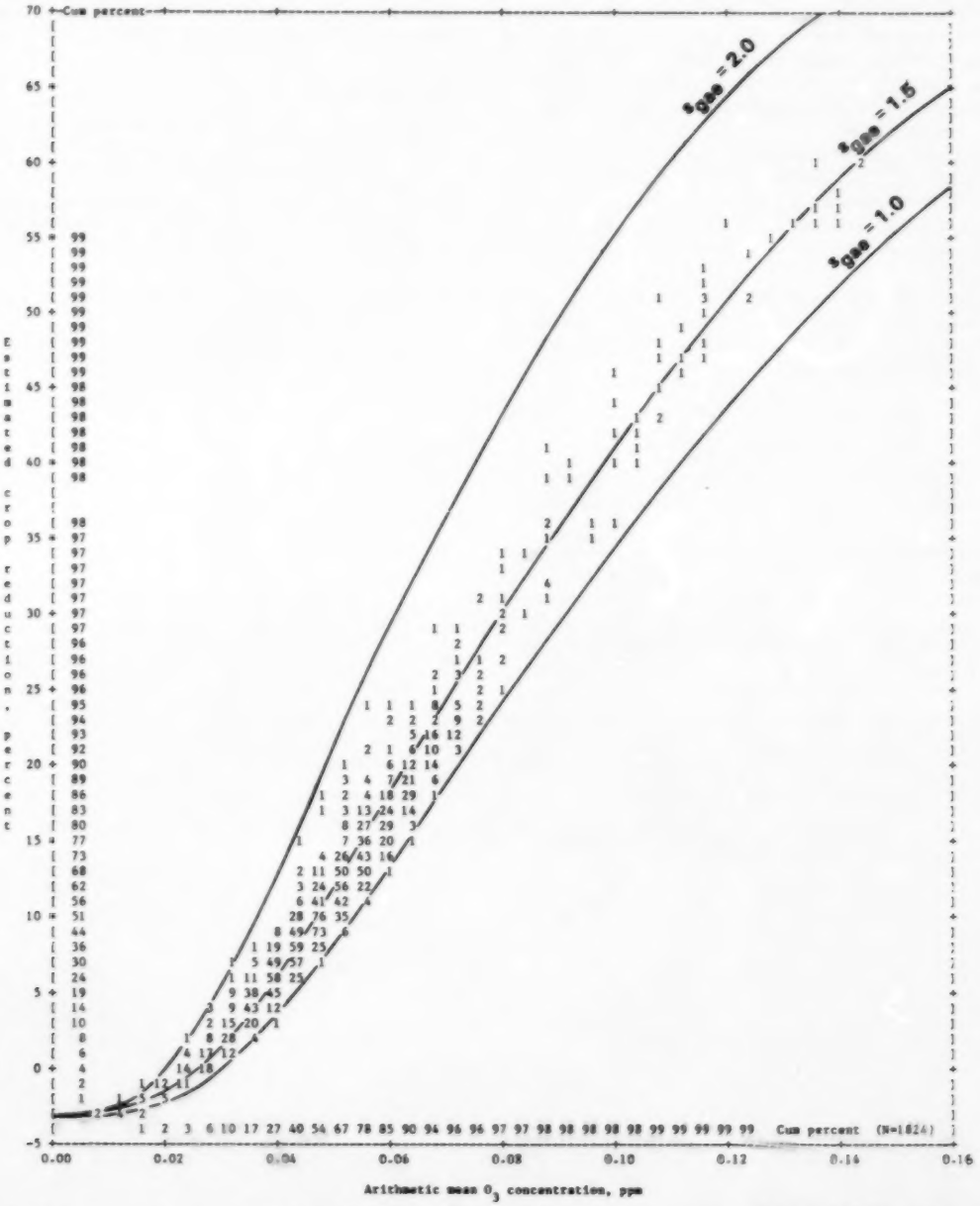

Figure 3. Number of site-years at estimated soybean percent crop reduction (for a 75-day exposure) versus 9:00 A.M.–4:00 P.M. arithmetic mean O_3 concentration measured at NADB sites for June 1–August 31 of each year, 1981-1983.

This rounds to 5 percent (first set of values).

The 4.8 percent crop reduction also is shown (Figure 2, top line) as a crop yield of 95.2 percent (100 − 4.8). Equation 4 is also rearranged and depicted there in a general lognormal form:

$$c_p = m_{gp} s_{gp}^{\ z} \tag{17}$$

$$c_p = (0.1317 \text{ ppm}) 2.197^{-1.670}$$

$$c_p = 0.0354 \text{ ppm}$$

where the p subscripts indicate plant effects lognormal parameters as compared with ambient air lognormal parameters (Equation 8).

The effective mean concentration can be estimated (second and third sets of values) from the two characteristic parameters of a lognormal distribution by applying, in order, Equations 11, 9, 10, and 12:

$$m_e = m_{ga} s_{ga}^{\ -(0.5/v) \ln s_{ga}} \tag{18}$$

Crop reduction can then be estimated (Equation 4). If the two characteristic parameters of a lognormal distribution are calculated when concentrations below 0.020 ppm are truncated, and an effective mean is estimated, then a 5 percent crop reduction is calculated (second set of values). If all the O_3 concentration data are used (third set of values), estimated crop reduction rises to 7 percent. Thus, for this set of concentration data, both the direct effective mean (first set) and the truncated distribution (second set) give the same estimated crop reduction, but using the entire concentration distribution (third set) results in a higher estimated crop reduction.

An estimate of crop reduction closer to that estimated with the measured m_e results if the measured arithmetic mean instead of the calculated geometric mean is used, by applying Equations 18 and 8:

$$m_e = m_a s_{ga}^{\ -0.5(1+1/v) \ln s_{ga}} \tag{19}$$

$$m_e = 0.0405 \text{ ppm}$$

A crop reduction of 6.6 percent is estimated (Equation 4) using the measured arithmetic mean, compared to 7.3 percent using the calculated geometric mean.

Equation 19 was substituted into Equation 4 to estimate soybean crop reduction as a function of the measured arithmetic mean and the effective ambient standard geometric deviation and to superimpose s_{gae} isopleths (Figure 3) on a previous plot (Figure 7 in Reference 2). On this plot 0 percent crop reduction is assumed at an assumed natural effective mean concentration of 0.030 ppm (comparable to an arithmetic mean approximating 0.025 ppm). (The natural effective mean concentration is the O_3 concentration expected due only to natural sources, from photochemically-reacted hydrocarbons emitted from trees, for instance.)

For the three year period plotted, 85 percent of the site-years are at or below an arithmetic mean of 0.06 ppm (bottom line of plot). The values below this concentration plot between the s_{gae} isopleths of 1.0 and 2.0. The greatest number of points for all concentrations plot near an s_{gae} of 1.5.

Summary

The two dashed lines in Figure 2 can be used to summarize and depict the calculations shown here. The mean impact of 0.000138 (point A) translates to an effective mean ambient O_3 concentration of 0.0354 ppm (point B) which reduces soybean crop yield an estimated 4.8 percent (point C).

Ambient air quality is characterized here only in terms of its expected effects on plants. An effective geometric mean and an effective standard geometric deviation are calculated from the effective and arithmetic means of an ambient air quality data set. These parameters are then used (Figure 3) as one example, to express estimated crop reduction as a function of the arithmetic mean O_3 concentration and the effective standard geometric deviation.

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